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A Jacobi-Galerkin Spectral Method for Computing the Ground and First Excited States of Nonlinear Fractional Schrödinger Equation

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Abstract. The behaviour of the ground and first excited states of the nonlinear fractional Schrödinger equation is studied by an approximation method. In order to determine the nonlinear term of the problem under consideration, a normalised fractional gradient flow is introduced and the decay of a modified energy is established. The problem is then discretised by a semi-implicit Euler method in time and Jacobi-Galerkin spectral method in space. One- and two-dimensional numerical examples show that the strong nonlocal interactions lead to a large scattering of particles. Moreover, numerical simulations confirm the fundamental gap conjecture and show that for small interactions the ground and first excited states are more peaked and narrower.

AMS subject classifications: 65N25, 65N30, 65N35

Key words: Fractional Schrödinger equation, semi-implicit Euler method, ground state, first excited state.

1. Introduction

The nonlinear Schrödinger equation is a fundamental model in many areas of physics, including quantum mechanics, fluids and nonlinear optics [31]. In order to extend Feynman path integral to Lévy one, Laskin [35,36] introduced a fractional Schrödinger equation. In dimensionless form the nonlinear fractional Schrödinger equation (NFSE) is

$$\left(D_{\mathbf{x}}^{\alpha} + V(\mathbf{x}) + \beta|\upsilon(\mathbf{x},t)|^2\right)\upsilon(\mathbf{x},t) = i\partial_t \upsilon(\mathbf{x},t), \quad \mathbf{x} \in \Omega \subseteq \mathbb{R}^d, \tag{1.1}$$

where $\mathbf{x} = (x, y)$, $\upsilon(\mathbf{x})$ is a complex-valued wave function, α the order of the fractional derivative, $V(x)$ the potential, and β the strength of the local (or short-range) interaction

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between particles. In this work we deal with repulsive interactions where $\beta \geq 0$. Besides, we assume that $\Omega = (-L, L)^d$, $d = 1, 2$.

The Riesz fractional operator $D_{\mathbf{x}}^{\alpha}$ is defined by

$$D_{\mathbf{x}}^{\alpha} \upsilon = \mathscr{F}^{-1}\left(\sum_{j=1}^{d} |k_j|^{\alpha} (\mathscr{F}\upsilon)(\mathbf{k})\right), \quad \mathbf{x}, \mathbf{k} \in \mathbb{R}^d, \quad \alpha \in (0, 2], \tag{1.2}$$

where

$$\mathscr{F}(g)(k) = \int_{\mathbb{R}} g(x) e^{-ikx} dx, \quad x, k \in \mathbb{R}$$

is the Fourier transform of the function $g(x)$, $\mathscr{F}^{-1}$ refers to the inverse Fourier transform, and $\mathbf{k} = (k_1, k_2)$, $d = 1, 2$. In one dimensional case and homogeneous Dirichlet boundary conditions, the Riesz fractional operator is equivalent to the fractional Laplacian $-(-\Delta)^{\alpha/2}$ [41, 43, 57], but for other dimensions, these operators are not equivalent.

In recent years, the computation of eigenvalues and eigenfunctions became an important problem in such areas as fluid mechanics, environmental studies, optics and electromagnetics [2, 7, 26, 56]. For various differential operators, a number of estimates and approximations have been obtained for eigenvalues [6, 25, 29, 30, 34, 37], eigenfunctions [11, 39, 61] and for the fundamental gap [16, 17, 33, 48]. Recall that the last one is referred to the difference between the two smallest eigenvalues. In physics literature, the eigenfunctions are called stationary states, the eigenfunction corresponding to the smallest nonzero eigenvalue is the ground state and the one corresponding to the larger eigenvalue is the excited state [28].

To compute the stationary states of (1.1), we write the wave function in the form

$$\upsilon(\mathbf{x}, t) = e^{-i\lambda t} u(\mathbf{x}), \quad \mathbf{x} \in \Omega \subseteq \mathbb{R}^d$$

and substitute it into the Eq. (1.1) equipped with specified boundary/initial conditions. The main purpose of this work is to provide satisfactory approximations for the ground and first excited states of the nonlinear fractional Schrödinger equation (NFSE).

More exactly, we consider the following time-independent nonlinear fractional Schrödinger equation (NFSE): Find a $\lambda \in \mathbb{R}$ and a real-valued wave function $u(\mathbf{x})$ such that

$$\begin{aligned} &\left(D_{\mathbf{x}}^{\alpha} + V(\mathbf{x}) + \beta |u(\mathbf{x})|^2\right) u(\mathbf{x}) = \lambda u(\mathbf{x}), \quad \mathbf{x} \in \Omega \subseteq \mathbb{R}^d, \\ &u(\mathbf{x}) = 0, \quad \mathbf{x} \in \Omega^c = \mathbb{R}^d / \Omega \end{aligned} \tag{1.3}$$

and

$$\|u\|^2 = \int_{\Omega} |u(\mathbf{x})|^2 d\mathbf{x} = 1. \tag{1.4}$$

We also assume that $V(\mathbf{x})$ is a real-valued harmonic trapping potential — i.e.

$$V(\mathbf{x}) = \begin{cases} \dfrac{1}{2}\gamma_x^2 x^2, & d = 1, \\ \dfrac{1}{2}\left(\gamma_x^2 x^2 + \gamma_y^2 y^2\right), & d = 2, \end{cases}$$